Mechanism of glycoside hydrolysis: A comparative QM/MM molecular dynamics analysis for wild type and Y69F mutant retaining xylanases†

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Electronic Supplementary Information

Cartesian coordinates (Ångström) for QM atoms of optimised geometries of key stationary structures

Wild Type BCX:
AM1/OPLS optimised geometry for reactant complex RC (QM atoms only, including Tyr69)

6	-2.459142130	11.798632787	3.074310880
6	-2.406034800	10.945034384	4.365699776
6	-2.931720575	11.786390270	5.539138106
6	-2.099696449	13.081318643	5.585141131
6	-2.258710667	13.841598467	4.267689103
8	-3.267985399	9.838117223	4.191534479
8	-2.758456527	11.037214903	6.730827506
8	-2.579496003	13.845485878	6.679176532
8	-1.792719303	13.054562069	3.182371479
6	-1.262051670	8.552244415	-0.240497667
6	-0.926353185	9.823612102	-1.026522650
6	-1.007512984	11.091562821	-0.162303607
6	-2.205892762	11.101412913	0.799401743
6	-3.053456106	9.837650829	0.668845476
8	-1.143167062	12.175076956	-1.087815812
8	-1.641286542	11.160956096	2.114403501
8	-2.268825860	8.660264155	0.732332172
8	0.346523295	9.732397112	-1.617682327
1	-3.522323532	11.943998380	2.740551016
1	-1.355756644	10.606552648	4.574797482
1	-4.024113486	12.019239851	5.400324284
1	-1.016481299	12.822698057	5.744698075
1	-1.607182692	14.755085381	4.248730730
1	-3.331524644	14.129281174	4.108359185
1	-2.788745187	9.205990171	3.634453515
1	-2.927781539	11.650130957	7.458991567
1	-1.964274526	14.583705303	6.780336733
1	-0.351735994	8.134381643	0.279608375
1	-1.644230799	9.893975541	-1.889445706
1	-0.048682241	11.202674204	0.421076077
1	-2.848655162	12.004776869	0.605171006
1	-3.637340721	9.867064917	-0.286736181
1	-3.735812912	9.739751018	1.558071449
1	-1.008735013	12.989325940	-0.586399810
1	0.992395664	9.395182913	-0.957527751
8	-1.833355949	7.622433448	-1.185682464
6	-1.208469276	6.386970780	-1.151415195
6	0.190277628	6.296945248	-1.187314915
6	-2.013261542	5.239508981	-1.095168154
1	0.813868459	7.205609502	-1.299793095
1	-3.105479627	5.327284109	-1.151906951
6	0.795750979	5.060097513	-1.024443471
6	-1.412685196	3.997284540	-0.937803092
1	1.897299009	4.976961498	-1.015451671
1	-2.025158957	3.085418855	-0.852817659
6	-0.014564207	3.924856515	-0.855095012
7	0.641910325	2.637855526	-0.553091704
8	-0.004860297	1.621314606	-0.576966154
8	1.805191394	2.645962413	-0.266926350
7	-6.476165021	1.039440738	-2.851768137
1	-6.377623266	0.245273883	-3.481065709
6	-6.554527655	2.336572123	-3.538106534
1	-7.185370919	3.017269907	-2.962804063

6	-5.148528919	2.961856844	-3.687614029
1	-4.687304916	2.996009683	-2.663276680
1	-4.488787703	2.297832110	-4.302147967
6	-5.134157502	4.359499843	-4.265311972
1	-5.365991399	4.345366193	-5.364563658
1	-5.892915186	5.010343472	-3.750402027
6	-3.782635034	4.988041341	-4.119488968
8	-2.683894631	4.601353826	-4.535462748
8	-3.790421320	6.172281079	-3.446050469
1	-2.878635611	6.475437052	-3.275993637
6	-7.226969128	2.087371919	-4.898708106
8	-7.203282486	0.963907505	-5.427655702
7	7.408585144	7.752080045	1.417970913
1	7.617798959	8.145044864	0.498266541
6	6.205530476	6.910182118	1.428201998
1	5.867332989	6.763955478	2.445965371
6	5.101543961	7.651405042	0.648765298
1	5.127633637	8.737828594	0.932618738
1	5.285047297	7.624546341	-0.453046615
6	3.713462115	7.145536003	0.930721427
1	3.596401745	6.086723702	0.578814710
1	3.535479917	7.172561606	2.036840943
6	2.631836981	7.959274418	0.249908508
8	2.728080075	8.316493416	-0.966860539
8	1.566787115	8.255494075	0.886251839
6	6.558162039	5.548806728	0.792383213
8	7.477877988	5.472993552	-0.038335478
7	0.984496382	-0.341681767	2.405180911
1	0.618029060	-0.789214711	3.256320822
6	1.238779073	1.082078075	2.521833189
1	1.851282728	1.421425651	1.690070526
6	-0.137260809	1.796706476	2.522130469
1	-0.682225961	1.541023789	1.615891719
1	-0.729442944	1.377246612	3.329426744
6	-0.171351084	3.315206690	2.670097638
6	0.952701043	4.101592938	2.343263005
1	1.870156960	3.671297556	1.968671684
6	-1.354397805	3.959720510	3.099308869
1	-2.236182715	3.380550964	3.330514769
6	0.902770869	5.493683815	2.462301462
1	1.786392866	6.060708875	2.238092874
6	-1.409062924	5.367783250	3.185808366
1	-2.325112588	5.863316531	3.469543907
6	-0.282697946	6.133916052	2.838797103
8	-0.322183184	7.494053914	2.837355297
1	-0.412917462	7.821961745	1.927371639
6	1.972886228	1.335765299	3.846026090
8	1.534882460	0.865476011	4.900534143

Wild Type BCX:
AM1/OPLS optimised geometry for transition structure TS1 (QM atoms only, including Tyr69)

6	-2.303326202	11.088693797	2.645651721
6	-2.278433547	10.461825389	4.060699320
6	-2.742465228	11.514967514	5.075993173
6	-1.855513318	12.762083413	4.900772298
6	-1.958443412	13.287494813	3.467244514
8	-3.200412693	9.391331160	4.079778631
8	-2.580911426	10.963953103	6.374246938
8	-2.325736141	13.723801306	5.832742847
8	-1.553149227	12.296084757	2.534293071
6	-0.233141172	8.362293380	-1.005660842
6	-0.303877328	9.780130147	-1.483939749
6	-0.729083009	10.733873541	-0.354574747
6	-1.930355293	10.204033899	0.444005209
6	-2.286284454	8.762646760	0.092201522
8	-1.079839085	11.962629013	-0.989807051
8	-1.562699575	10.213763225	1.824200700
8	-1.143811112	7.914309113	-0.147996801
8	0.906243438	10.219874817	-2.040158051
1	-3.353407819	11.251926813	2.290719290
1	-1.242827649	10.107405122	4.312875982
1	-3.825069103	11.773723244	4.912236641
1	-0.787405123	12.495592720	5.130387186
1	-1.243280818	14.135681109	3.297451795
1	-3.008808582	13.616772744	3.248769002
1	-2.764507845	8.652328406	3.632032625
1	-2.717953725	11.693456872	6.992043993
1	-1.717792659	14.472499277	5.786982323
1	0.524124178	7.636424980	-1.367307907
1	-1.048584372	9.794847731	-2.334242963
1	0.146081693	10.885046254	0.342908148
1	-2.831016957	10.853148219	0.254057800
1	-2.924641448	8.726808336	-0.829571833
1	-2.785833282	8.257911190	0.964768252
1	-1.065182825	12.640831667	-0.299790682
1	1.631875829	9.954635209	-1.446334430
8	-1.297900008	7.562951616	-2.665426818
6	-1.303052127	6.292207354	-2.408617093
6	-0.095625815	5.558452802	-2.175100504
6	-2.534252287	5.584442043	-2.259309278
1	0.868739505	6.013225027	-2.444566103
1	-3.463592615	6.105890083	-2.523113554
6	-0.124464471	4.284400007	-1.660101458
6	-2.567175616	4.315784552	-1.729901656
1	0.815101879	3.739071787	-1.463200006
1	-3.529779705	3.811651256	-1.540851519
6	-1.364525830	3.663865966	-1.391206451
7	-1.415152619	2.356609504	-0.752939721
8	-2.475297454	1.945294422	-0.333415382
8	-0.416378809	1.687591037	-0.646852597
7	7.041091351	7.958961618	1.436801637
1	7.247326182	8.364189742	0.528160813
6	5.836639363	7.120995228	1.470623326
1	5.522871832	6.944956627	2.492595545

6	4.712697869	7.881184634	0.745699773
1	4.687829427	8.931896438	1.141110226
1	4.945470668	7.967744909	-0.347742853
6	3.330196222	7.297928977	0.904869752
1	3.299310564	6.238456273	0.535337135
1	3.008354792	7.295675682	1.975340810
6	2.347856867	8.070363642	0.060736850
8	2.594294737	8.291952417	-1.162450993
8	1.213865755	8.482607516	0.524939143
6	6.174451580	5.784947185	0.782281357
8	7.101752004	5.727880754	-0.035187063
7	-6.492270546	1.036303377	-2.950457781
1	-6.329295110	0.235618730	-3.550246112
6	-6.646760799	2.305259158	-3.669173037
1	-7.227591004	3.010623565	-3.071271438
6	-5.263912303	2.918521125	-3.980668820
1	-4.726840749	3.060146975	-3.003253180
1	-4.645355987	2.192587047	-4.565837022
6	-5.304437446	4.248780100	-4.698187553
1	-5.818475319	4.176595270	-5.694050033
1	-5.848614898	5.007387888	-4.073706560
6	-3.930227835	4.752916366	-5.007886259
8	-2.964925431	4.138906843	-5.473631066
8	-3.772973074	6.089886867	-4.800050954
1	-2.830040242	6.329820949	-4.861484166
6	-7.416699913	1.995793136	-4.961147207
8	-7.347067979	0.881582932	-5.494322667
7	0.776571775	-0.316940670	2.640480395
1	0.464223283	-0.742557941	3.515636642
6	0.945989746	1.124754688	2.673398146
1	1.520400572	1.448234312	1.809714821
6	-0.458348867	1.764104184	2.647299461
1	-1.017366006	1.386209078	1.795216944
1	-1.012319849	1.420707354	3.514947735
6	-0.499129414	3.284603083	2.610835513
6	0.348646723	3.990750685	1.734020617
1	1.004099325	3.466798401	1.053004416
6	-1.383631227	4.001924382	3.444582512
1	-2.066306107	3.478208454	4.095387895
6	0.330090266	5.393382957	1.705943884
1	0.962497009	5.905709590	1.002036337
6	-1.388923910	5.411181108	3.423085187
1	-2.060348035	5.967254961	4.056655371
6	-0.519912204	6.106311197	2.566427188
8	-0.505165906	7.467571857	2.571540320
1	-0.037207122	7.811280296	1.802034034
6	1.677144124	1.506580775	3.965188580
8	1.373832530	0.975139159	5.034337206

Wild Type BCX:
AM1/OPLS optimised geometry for intermediate INT (QM atoms only, including Tyr69)

6	-2.427490282	11.385400867	2.905657215
6	-2.391405663	10.657401191	4.274143005
6	-2.965449686	11.589436776	5.355633143
6	-2.192491895	12.915391757	5.275898576
6	-2.389747647	13.534147011	3.890242601
8	-3.234656912	9.526130580	4.210782462
8	-2.773251603	10.967232814	6.617435841
8	-2.670025124	13.766156471	6.304624900
8	-1.808368094	12.672148746	2.922887967
6	-0.120254058	8.743232988	-0.556095363
6	-0.402475595	10.097677530	-1.208259589
6	-0.863042628	11.165679628	-0.209659853
6	-2.002732602	10.617646970	0.671710859
6	-2.293730166	9.147160371	0.372071331
8	-1.341005637	12.255424016	-0.995022906
8	-1.569473436	10.683891661	2.036172566
8	-1.122046927	8.341814354	0.352430343
8	0.736089037	10.603673822	-1.868366890
1	-3.481639566	11.470492064	2.536546687
1	-1.338493343	10.361794102	4.528302770
1	-4.065199724	11.755430371	5.186392818
1	-1.098875189	12.707727177	5.434282802
1	-1.831070882	14.499950072	3.786429806
1	-3.479020804	13.695706299	3.675986996
1	-2.791737724	8.880452409	3.642355360
1	-3.017111067	11.627700684	7.279713384
1	-2.006040199	14.462010397	6.396323623
1	-0.015829147	7.941296671	-1.348082938
1	-1.218322459	9.899540892	-1.961398192
1	0.003758797	11.490157673	0.429775398
1	-2.934237077	11.224403602	0.500793007
1	-2.834235984	9.056861994	-0.606049366
1	-2.904277465	8.687015566	1.198244434
1	-1.325395723	13.035618400	-0.424229508
1	1.063359335	9.885702840	-2.434657592
8	-0.380757328	8.144865012	-4.212339535
6	-0.740636319	7.080454475	-3.610408691
6	0.160002135	6.335520436	-2.767615707
6	-2.083293884	6.573804259	-3.716169049
1	1.209175062	6.655961836	-2.718724059
1	-2.771035106	7.094128114	-4.394090588
6	-0.237516839	5.208611609	-2.096022523
6	-2.472180960	5.441937600	-3.046584617
1	0.483988296	4.636127899	-1.487923816
1	-3.501457354	5.058167222	-3.160788321
6	-1.570872838	4.746638651	-2.209843336
7	-1.984567888	3.534028928	-1.521228175
8	-3.123451451	3.132895812	-1.626246828
8	-1.190634258	2.917279173	-0.851670496
7	-6.730445741	0.868616951	-2.289787298
1	-6.470345217	0.040025544	-2.813932148
6	-6.825543543	2.103221033	-3.072379966
1	-7.057816958	2.951365519	-2.427435469

6	-5.503767360	2.388401341	-3.815026082
1	-4.678594357	2.475620971	-3.054591777
1	-5.231793627	1.529517904	-4.476899880
6	-5.539804922	3.653635559	-4.640368364
1	-6.229568545	3.558061008	-5.522301125
1	-5.893359113	4.518441320	-4.016760001
6	-4.205594068	4.002507254	-5.207109407
8	-3.186843704	3.314502606	-5.313778722
8	-4.139838522	5.277767045	-5.686164848
1	-3.230380044	5.482898018	-5.968643575
6	-7.943475042	1.914708706	-4.100245879
8	-8.092726911	0.835514122	-4.684897967
7	6.901619961	8.282316047	1.160229245
1	7.075360930	8.717799643	0.259086502
6	5.696740082	7.443688546	1.212264293
1	5.403150981	7.271532137	2.245068232
6	4.565137514	8.201971059	0.483335171
1	4.571661601	9.267138012	0.840506981
1	4.784720607	8.237498440	-0.616350908
6	3.175388158	7.654227244	0.699976500
1	3.129751313	6.551077414	0.481091960
1	2.841322916	7.803418214	1.759722635
6	2.206814136	8.296706988	-0.246686811
8	2.354541459	8.465491633	-1.462184546
8	1.026528507	8.722318001	0.311510793
6	6.040733488	6.107827688	0.523241725
8	6.870554566	6.088922105	-0.395209553
7	0.827767105	0.109922312	2.637127624
1	0.487860475	-0.299786807	3.508879543
6	0.925250089	1.557137877	2.628119877
1	1.541036086	1.894859993	1.795584596
6	-0.501878511	2.126525511	2.482562640
1	-0.912875730	1.830167332	1.517068433
1	-1.153681479	1.678842098	3.228985111
6	-0.591618487	3.637493773	2.584885611
6	0.112317506	4.428186761	1.658973197
1	0.641293000	3.966227346	0.836439135
6	-1.286594672	4.256728830	3.645973977
1	-1.857365079	3.668085873	4.343192809
6	0.136252427	5.822436763	1.804011868
1	0.672650349	6.399385225	1.074759403
6	-1.269416602	5.658054684	3.780017295
1	-1.825353380	6.140630157	4.567405681
6	-0.544228235	6.440525746	2.868582116
8	-0.551778835	7.797026542	2.986398277
1	-0.403166839	8.188404761	2.123749684
6	1.571692750	2.006491213	3.944732372
8	1.334523736	1.412850130	4.999834026

Tyr69/Phe mutant BCX:
AM1/OPLS optimised geometry for reactant complex RC (QM atoms only, including Phe69)

6	-2.584231584	11.689631374	2.783904799
6	-2.515362991	10.945279033	4.138161483
6	-3.056513443	11.858893718	5.246872544
6	-2.284414087	13.189781752	5.183473518
6	-2.447086128	13.822913793	3.799916746
8	-3.366971304	9.818419023	4.046157354
8	-2.831163474	11.210485579	6.488837547
8	-2.823009235	14.019586151	6.199589094
8	-1.933600101	12.958279087	2.796825378
6	-1.219520080	8.329342300	-0.532673644
6	-0.979462483	9.641165228	-1.294280546
6	-1.098724932	10.874267643	-0.383414039
6	-2.304319337	10.826752927	0.567032934
6	-3.049749597	9.497769598	0.469434407
8	-1.255416288	11.989937519	-1.265410721
8	-1.763593640	10.975706100	1.884058551
8	-2.171773189	8.386257499	0.503299437
8	0.275846115	9.656680238	-1.926634563
1	-3.647649882	11.796330575	2.439956382
1	-1.458127450	10.638852703	4.365957440
1	-4.159796392	12.035530486	5.110292827
1	-1.194432590	12.997945266	5.384708705
1	-1.830231856	14.755313414	3.705574208
1	-3.526811562	14.055406849	3.600828358
1	-2.868011735	9.141312823	3.568753515
1	-3.066340745	11.852729894	7.171838764
1	-2.298628793	14.830687838	6.196199671
1	-0.274758534	7.912335139	-0.068754286
1	-1.732480475	9.706406003	-2.129234089
1	-0.144738734	10.981617667	0.206830362
1	-3.014682920	11.668496508	0.332605668
1	-3.661865664	9.486016817	-0.469653393
1	-3.702610943	9.350303236	1.373485715
1	-1.149681097	12.786771318	-0.730657036
1	0.937361572	9.225446601	-1.342896135
8	-1.821388777	7.441448192	-1.491361005
6	-1.439253383	6.117563590	-1.370302309
6	-0.103147809	5.725720321	-1.218342372
6	-2.465968440	5.163541982	-1.473912163
1	0.713871216	6.473642450	-1.240156110
1	-3.490439698	5.478705048	-1.701218605
6	0.194946676	4.378155241	-1.039459472
6	-2.181384235	3.824647372	-1.270787427
1	1.241797209	4.049893364	-0.912130612
1	-2.987991342	3.073530751	-1.292524316
6	-0.853962661	3.444912691	-1.012835884
7	-0.580326228	2.033165856	-0.697774910
8	-1.505941715	1.317288948	-0.397982862
8	0.541597771	1.612005945	-0.726423131
7	-6.601599462	1.241481538	-3.092146386
1	-6.509913485	0.452478549	-3.726952895
6	-6.719849775	2.533795593	-3.778427249
1	-7.370941576	3.196671673	-3.204687666

6	-5.333546889	3.200654518	-3.934406565
1	-4.875210670	3.268382496	-2.909488688
1	-4.651904659	2.545630122	-4.534306759
6	-5.357725818	4.587100168	-4.538758729
1	-5.629526564	4.551139468	-5.628415887
1	-6.104048858	5.238427603	-4.007465879
6	-4.006893956	5.228003965	-4.458868245
8	-2.924661607	4.840840744	-4.914587639
8	-3.989240384	6.423409817	-3.803461142
1	-3.070962928	6.727323911	-3.673750826
6	-7.385765853	2.249095972	-5.135475355
8	-7.327455372	1.120824873	-5.653036140
7	7.199226209	7.875672229	1.283010397
1	7.411660521	8.226158612	0.346812961
6	6.032283126	6.985363312	1.313720569
1	5.727316141	6.793587497	2.335416027
6	4.874831065	7.682431679	0.572378404
1	4.701553329	8.683265126	1.051918798
1	5.157713835	7.895579401	-0.490060055
6	3.567201850	6.932820132	0.582041091
1	3.652750225	5.966283003	0.020937997
1	3.266436823	6.705101899	1.636652548
6	2.474997266	7.742706698	-0.083859024
8	2.425501275	7.856280341	-1.348909714
8	1.558857634	8.288391372	0.614484529
6	6.410924379	5.652629555	0.644448013
8	7.305292420	5.608816331	-0.215852274
7	0.937066320	-0.318664634	2.477871374
1	0.496835944	-0.712768901	3.319283821
6	1.140940250	1.117794722	2.538351638
1	1.639507343	1.476923846	1.640111878
6	-0.274928296	1.725712076	2.681519135
1	-0.935382739	1.307259840	1.930380981
1	-0.686250933	1.360391791	3.616487672
6	-0.466915892	3.237782056	2.686109748
6	0.542072796	4.125116827	2.254796632
1	1.484161488	3.769382349	1.861528566
6	-1.719375609	3.760717927	3.074098068
1	-2.524218895	3.095080942	3.347702253
6	0.309439506	5.510111659	2.250209638
1	1.081032799	6.169296818	1.887926382
6	-1.950468746	5.148975867	3.060674572
1	-2.920821724	5.540771763	3.323246737
6	-0.935971065	6.027607363	2.644645623
1	-1.120804341	7.091256531	2.587589245
6	1.944477683	1.446044892	3.804607541
8	1.650115472	0.910685488	4.880925878

Tyr69/Phe mutant BCX:
AM1/OPLS optimised geometry for transition structure TS1 (QM atoms only, including Phe69)

6	-2.429847099	11.374820958	2.768046628
6	-2.511777530	10.830525605	4.211897885
6	-3.032107945	11.924452234	5.151513868
6	-2.183268662	13.192618488	4.947617361
6	-2.210326529	13.622437371	3.478809708
8	-3.457094010	9.778395976	4.209395272
8	-2.888774928	11.435617383	6.477361880
8	-2.751093969	14.187876788	5.785032329
8	-1.698353055	12.591854223	2.644230563
6	0.180262351	8.877701803	-0.765888202
6	-0.039607176	10.304229552	-1.180259009
6	-0.530520341	11.119871669	0.028344593
6	-1.774166421	10.460066793	0.654035912
6	-1.956914831	9.007649664	0.221231529
8	-0.889700167	12.410884882	-0.448859768
8	-1.616658525	10.454847892	2.072256372
8	-0.720974649	8.293390192	0.016278534
8	1.065072822	10.921483027	-1.788120997
1	-3.450795900	11.492891092	2.318085183
1	-1.502305745	10.473173685	4.552975705
1	-4.116612243	12.141185301	4.945042412
1	-1.122730355	12.990172125	5.261817609
1	-1.523008560	14.491162988	3.299853691
1	-3.256349091	13.886542960	3.169303315
1	-2.997544557	9.004690814	3.857198322
1	-3.128141878	12.167886903	7.059057533
1	-2.211638785	14.981576937	5.678390066
1	0.987521368	8.222292895	-1.149097760
1	-0.840516630	10.264941692	-1.979756684
1	0.301529355	11.185819554	0.783789806
1	-2.693541166	11.039265119	0.354656395
1	-2.524586773	8.963552124	-0.747055336
1	-2.468800047	8.402978087	1.017228171
1	-0.841094375	13.009825236	0.311249489
1	1.878941041	10.574556582	-1.379793381
8	-0.647811176	8.137676602	-2.608345464
6	-0.782208447	6.864341396	-2.410815913
6	0.321827228	6.038963376	-2.022759215
6	-2.066005825	6.244791879	-2.495251657
1	1.340360346	6.445781907	-2.078222796
1	-2.907233774	6.851235166	-2.854374790
6	0.132062764	4.742008710	-1.609476956
6	-2.258849528	4.947316295	-2.079876637
1	0.989431669	4.118318409	-1.301061006
1	-3.262854247	4.492328557	-2.116300494
6	-1.172021196	4.196885515	-1.589688592
7	-1.391834214	2.851691093	-1.076089169
8	-2.522255149	2.473520668	-0.854432103
8	-0.454514128	2.119108135	-0.875215232
7	7.385460401	7.998904148	1.356261271
1	7.605117579	8.372071755	0.436253832
6	6.141685353	7.229150028	1.422885836
1	5.868863950	7.039529082	2.455370867

6	5.053817462	8.081801277	0.751690648
1	5.213762555	9.155482095	1.042764263
1	5.164507170	8.055687671	-0.363400726
6	3.632761264	7.736987446	1.113847847
1	3.383447038	6.679620899	0.834102700
1	3.474116102	7.848659252	2.213295009
6	2.679406419	8.627967296	0.357825451
8	2.938506175	8.990455194	-0.830219014
8	1.550310222	9.001504079	0.860391768
6	6.367145727	5.888897815	0.702717042
8	7.326887283	5.754718601	-0.068597628
7	-6.777422583	1.128216721	-3.079215789
1	-6.636560257	0.318339504	-3.673301764
6	-6.916747091	2.395828098	-3.801973194
1	-7.511021614	3.099278151	-3.215220226
6	-5.524832425	3.006465324	-4.069898750
1	-4.989412504	3.092568675	-3.084304102
1	-4.912799847	2.305715923	-4.692974901
6	-5.548697138	4.372265973	-4.715958705
1	-6.097167362	4.370549827	-5.695804656
1	-6.047175787	5.114300549	-4.036750662
6	-4.167086842	4.840082796	-5.042381222
8	-3.223518719	4.202352575	-5.521096311
8	-3.961754222	6.168374453	-4.822248734
1	-3.022360977	6.388091729	-4.969361373
6	-7.659731160	2.094060100	-5.113018344
8	-7.582005228	0.981915878	-5.647995964
7	0.673635552	-0.008715123	2.363708887
1	0.370602010	-0.418099264	3.249810750
6	0.834769855	1.436304747	2.372942963
1	1.396916887	1.759779196	1.499991509
6	-0.576741738	2.066058827	2.354467017
1	-1.117926968	1.729755156	1.473780429
1	-1.136445760	1.653947584	3.187551974
6	-0.684432734	3.586079491	2.429250554
6	0.303098370	4.421252615	1.861549510
1	1.143221355	4.005807511	1.324456599
6	-1.813420446	4.173237586	3.039978725
1	-2.608056391	3.549943777	3.422493339
6	0.201179952	5.819113170	1.973114014
1	0.964322404	6.451670457	1.543852257
6	-1.934728068	5.574933699	3.112522804
1	-2.823083071	6.023340402	3.527614063
6	-0.911531113	6.396906528	2.608411946
1	-0.985076651	7.472328896	2.677729120
6	1.574697297	1.803744905	3.665434785
8	1.237814520	1.295800976	4.737628944

Tyr69/Phe mutant BCX:
AM1/OPLS optimised geometry for intermediate INT (QM atoms only, including Phe69)

6	-2.451978428	11.250635229	2.787726377
6	-2.415893809	10.522635553	4.156212167
6	-2.989937832	11.454671138	5.237702305
6	-2.216980041	12.780626119	5.157967738
6	-2.414235793	13.399381373	3.772311763
8	-3.259145058	9.391364942	4.092851624
8	-2.797739749	10.832467176	6.499505003
8	-2.694513270	13.631390833	6.186694062
8	-1.832856240	12.537383108	2.804957129
6	-0.144742204	8.608467350	-0.674026201
6	-0.426963741	9.962911892	-1.326190427
6	-0.887530774	11.030913990	-0.327590691
6	-2.027220748	10.482881332	0.553780021
6	-2.318218312	9.012394733	0.254140493
8	-1.365493783	12.120658378	-1.112953744
8	-1.593961582	10.549126023	1.918241728
8	-1.146535073	8.207048716	0.234499505
8	0.711600891	10.468908184	-1.986297728
1	-3.506127712	11.335726426	2.418615849
1	-1.362981489	10.227028464	4.410371932
1	-4.089687870	11.620664733	5.068461980
1	-1.123363335	12.572961539	5.316351964
1	-1.855559028	14.365184434	3.668498968
1	-3.503508950	13.560940661	3.558056158
1	-2.816225870	8.745686771	3.524424522
1	-3.041599213	11.492935046	7.161782546
1	-2.030528345	14.327244759	6.278392785
1	-0.040317293	7.806531033	-1.466013776
1	-1.242810605	9.764775254	-2.079329030
1	-0.020729349	11.355392035	0.311844560
1	-2.958725223	11.089637964	0.382862169
1	-2.858724130	8.922096356	-0.723980204
1	-2.928765611	8.552249928	1.080313596
1	-1.349883869	12.900852762	-0.542160346
1	1.038871189	9.750937202	-2.552588430
8	-0.571623924	8.042242838	-4.278460672
6	-0.931502915	6.977832301	-3.676529828
6	-0.030864461	6.232898262	-2.833736844
6	-2.274160480	6.471182085	-3.782290186
1	1.018308466	6.553339662	-2.784845196
1	-2.961901702	6.991505940	-4.460211725
6	-0.428383435	5.105989435	-2.162143660
6	-2.663047556	5.339315426	-3.112705754
1	0.293121700	4.533505725	-1.554044953
1	-3.692323950	4.955545048	-3.226909458
6	-1.761739434	4.644016477	-2.275964473
7	-2.175434484	3.431406754	-1.587349312
8	-3.314318047	3.030273638	-1.692367965
8	-1.381500854	2.814656999	-0.917791633
7	-6.703602707	1.215545033	-2.219838522
1	-6.443502183	0.386953626	-2.743983372
6	-6.798700509	2.450149115	-3.002431190
1	-7.030973924	3.298293601	-2.357486693

6	-5.476924326	2.735329423	-3.745077306
1	-4.651751323	2.822549053	-2.984643001
1	-5.204950593	1.876445986	-4.406951104
6	-5.512961888	4.000563641	-4.570419588
1	-6.202725511	3.904989090	-5.452352349
1	-5.866516079	4.865369402	-3.946811225
6	-4.178751034	4.349435336	-5.137160631
8	-3.160000670	3.661430688	-5.243829946
8	-4.112995488	5.624695127	-5.616216072
1	-3.264173215	6.102629949	-5.608047499
6	-7.916632008	2.261636788	-4.030297103
8	-8.065883877	1.182442204	-4.614949191
7	6.877131815	8.147550409	1.042298407
1	7.050872784	8.583034005	0.141155664
6	5.672251936	7.308922908	1.094333455
1	5.378662835	7.136766499	2.127137394
6	4.540649368	8.067205421	0.365404333
1	4.547173455	9.132372374	0.722576143
1	4.760232461	8.102732802	-0.734281746
6	3.150900012	7.519461606	0.582045662
1	3.105263167	6.416311776	0.363161122
1	2.816834770	7.668652576	1.641791797
6	2.182325990	8.161941350	-0.364617649
8	2.330053313	8.330725995	-1.580115384
8	1.002040361	8.587552363	0.193579955
6	6.016245342	5.973062050	0.405310887
8	6.846066420	5.954156467	-0.513140391
7	0.792824798	0.384467169	2.710071788
1	0.452918168	-0.025241950	3.581823707
6	0.890307782	1.831682734	2.701064041
1	1.506093779	2.169404850	1.868528760
6	-0.536820818	2.401070368	2.555506804
1	-0.947818037	2.104712189	1.590012597
1	-1.188623786	1.953386955	3.301929275
6	-0.626560794	3.912038630	2.657829775
6	0.077375199	4.702731618	1.731917361
1	0.606350693	4.240772203	0.909383299
6	-1.321536979	4.531273687	3.718918141
1	-1.892307386	3.942630730	4.416136973
6	0.101310120	6.096981620	1.876956032
1	0.637708042	6.673930082	1.147703567
6	-1.304358909	5.932599541	3.852961459
1	-1.860295687	6.415175014	4.640349845
6	-0.579170542	6.715070603	2.941526280
1	-0.585057569	7.772702681	3.033384797
6	1.536750443	2.281036070	4.017676536
8	1.299581429	1.687394987	5.072778190

Wild-type BCX:
AM1 optimised geometry for transition structure TS1 (gas phase)

8	0.777288000	-0.755304000	1.212428000
6	0.930952000	-0.733102000	-0.111587000
6	1.899288000	0.221356000	-0.766346000
6	3.184472000	0.402019000	0.073539000
6	2.927206000	0.377974000	1.594725000
6	1.439106000	0.311178000	1.927021000
8	2.208938000	-0.200125000	-2.073915000
8	3.839955000	1.603281000	-0.284994000
8	3.629366000	-0.672473000	2.223313000
8	-0.619656000	0.502887000	-0.288788000
6	-1.845262000	0.103691000	-0.160639000
6	-2.918050000	0.989111000	-0.508833000
6	-4.230512000	0.605855000	-0.373955000
6	-4.548908000	-0.680843000	0.117740000
6	-3.509113000	-1.574381000	0.463863000
6	-2.195108000	-1.193078000	0.330766000
7	-5.943743000	-1.082254000	0.267921000
8	-6.213517000	-2.181306000	0.693280000
8	-6.827643000	-0.312046000	-0.030245000
8	2.461374000	-2.251265000	0.138652000
6	2.352467000	-3.266398000	-0.645959000
6	3.034216000	-4.562641000	-0.263854000
8	1.703045000	-3.138397000	-1.720047000
8	-0.571311000	3.389954000	-0.982615000
6	0.486367000	4.028812000	-0.435744000
6	0.529837000	5.497083000	-0.728160000
6	1.046402000	6.279380000	0.451256000
8	1.294964000	3.354093000	0.216268000
1	-0.542806000	2.428116000	-0.778954000
1	-1.385259000	-1.880772000	0.613646000
1	-3.761979000	-2.578535000	0.843844000
1	-5.044737000	1.297471000	-0.647675000
1	-2.664914000	1.987112000	-0.893347000
1	3.211836000	2.327788000	-0.158858000
1	3.355490000	1.314530000	2.057561000
1	1.273567000	0.036882000	3.000643000
1	1.394365000	1.229780000	-0.896385000
1	0.929726000	1.275667000	1.660287000
1	0.422034000	-1.545926000	-0.670414000
1	3.916098000	-0.414834000	-0.195183000
1	3.346046000	-1.506498000	1.812712000
1	2.417514000	-1.151581000	-2.039190000
1	1.204083000	5.637241000	-1.615885000
1	-0.495673000	5.847656000	-1.018624000
1	1.184292000	7.349842000	0.165927000
1	0.327430000	6.227760000	1.304172000
1	2.026543000	5.866247000	0.794390000
6	2.102921000	-5.737817000	-0.395585000
1	3.916250000	-4.695491000	-0.943312000
1	3.417754000	-4.482245000	0.785530000
1	2.656452000	-6.695840000	-0.245083000
1	1.286194000	-5.678668000	0.363605000
1	1.635780000	-5.743522000	-1.411014000

Wild-type BCX:
B3LYP/6-31G* optimised geometry for transition structure TS1 (gas phase)

6	1.455413000	-1.861868000	0.673358000
6	1.840519000	-0.570521000	0.196003000
6	3.159898000	-0.429645000	-0.337545000
6	4.029068000	-1.503316000	-0.385064000
6	3.619444000	-2.763528000	0.089697000
6	2.327306000	-2.934148000	0.618694000
8	1.016896000	0.442161000	0.246874000
7	4.524469000	-3.876736000	0.037395000
8	5.666358000	-3.700293000	-0.428993000
8	4.139871000	-4.983531000	0.460275000
6	-1.214432000	0.263414000	-0.229781000
8	-1.273027000	1.328917000	-0.950650000
6	-1.815483000	2.532844000	-0.314026000
6	-3.162035000	2.215570000	0.334427000
6	-3.007502000	1.077134000	1.368510000
6	-1.683077000	0.277518000	1.202126000
8	-1.746309000	-0.992946000	1.784961000
8	-3.047595000	1.654772000	2.677005000
8	-4.145091000	1.936152000	-0.645310000
8	-3.266477000	-0.616708000	-1.091584000
6	-3.803194000	-1.726022000	-0.742194000
6	-4.838286000	-2.304126000	-1.716207000
6	-5.511269000	-3.596831000	-1.252812000
8	-3.534696000	-2.351284000	0.313570000
8	1.466066000	2.985846000	0.308959000
6	2.480505000	3.581544000	-0.315864000
6	2.463295000	5.090290000	-0.102701000
6	3.615010000	5.820831000	-0.791984000
8	3.326730000	3.002383000	-0.978886000
1	1.447364000	1.965082000	0.185776000
1	-0.877275000	-0.627621000	-0.735630000
1	-0.908936000	0.838556000	1.742022000
1	-1.068818000	2.894856000	0.399339000
1	-2.896977000	0.932778000	3.310844000
1	-3.842523000	0.381893000	1.242378000
1	-3.492764000	3.112021000	0.870664000
1	-3.973859000	1.026756000	-0.991172000
1	-1.924893000	3.239343000	-1.135962000
1	3.462940000	0.545901000	-0.707129000
1	5.028376000	-1.391140000	-0.790908000
1	2.031354000	-3.909983000	0.987483000
1	0.465471000	-1.976757000	1.106237000
1	-2.411862000	-1.547373000	1.273393000
1	1.491796000	5.463414000	-0.454527000
1	2.470943000	5.270108000	0.980750000
1	3.551941000	6.899914000	-0.604940000
1	4.583020000	5.462246000	-0.426862000
1	3.595154000	5.655069000	-1.874160000
1	-5.583534000	-1.519456000	-1.905743000
1	-4.323304000	-2.454118000	-2.675132000
1	-6.228243000	-3.951091000	-2.005576000
1	-4.771503000	-4.385421000	-1.080681000
1	-6.048050000	-3.446415000	-0.309810000